

WHAT IS CLAIMED IS:

1. A method of separating a compound of interest from a mixture, the method comprising the steps of:

- (a) providing a mixture containing a compound of interest;
- (b) subjecting a portion of the mixture to a separation using thin layer chromatography to determine an R_f value for the compound of interest;
- (c) predicting an elution time of the compound of interest on a preparative scale HPLC column using the determined R_f value for the compound of interest;
- (d) subjecting all or a portion of the remaining mixture to a preparative scale HPLC system comprising a preparative scale HPLC column; and
- (e) collecting at least a portion of the compound of interest using the predicted elution time.

2. The method of claim 1 wherein the step of predicting an elution time for the compound of interest comprises:

- (1) predicting a retention time of the compound of interest from the preparative scale HPLC column using a predetermined correlation function between R_f value from the TLC and retention time on the preparative scale HPLC column along with the determined R_f value of the compound of interest; and
- (2) selecting a window of time around the predicted retention time within which the compound is expected to elute.

3. The method of claim 1 wherein step (b) comprises:

- (1) subjecting a portion of the mixture to a separation using thin layer chromatography to produce one or more spots or zones;
- (2) analyzing the one or more spots or zones using a mass spectrometer to determine the spot or zone containing the compound of interest; and
- (3) determining an R_f value for the compound of interest.

4. The method of claim 1 wherein an artificial neural network is used to predict the elution time in step (c).

5. The method of claim 1 wherein a dynamic correlation function is used to predict the elution time in step (c).